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Multiburst and Fratricide Effects
Task One: Numerical Methods and Computational Results

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Technical Report

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13. ABSTRACT *(Maximum 200 words)*

This report documents and summarizes several developments in the field of numerical analysis of systems of hyperbolic conservation laws (especially, gas dynamics) and their viscous extensions (especially, the Navier-Stokes equations); applications of the methods obtained in large-scale scientific computing with the objective of modeling complex physical phenomena, including careful checks against experimental data; and further applications of the methodology in the modeling of blast wave environments. Of special note are results concerning shear layer and boundary layer phenomenology (the latter including the effects of dust, preheating, etc.) and new methods for multimaterial calculations and problems involving wave speed stiffness (e.g., the early stages of fireball rise).

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SECTION 1
INTRODUCTION

The prediction of blast wave environments, whether a result of a chemical or a nuclear source, is an extremely challenging technical problem. A combination of analytical reasoning, study of the records of nonrepeatable historical events, design and study of (perhaps) repeatable large-scale field simulations, laboratory experiments and studies involving computational fluid dynamics (CFD) are all involved in a highly interactive and fast-changing dynamic process. Among the difficulties encountered are (1) the problems posed are often three-dimensional whereas simulations are more easily arranged for two-dimensional analysis, (2) many unusual physical phenomena must be dealt with including, but not limited to, high temperature real gas effects, very strong incident shock waves, rapid fireball rise leading to a multiscale flowfield, complex and unusual multiphase boundary layer effects including cratering and precursor/decursor effects in certain situations and (3) the necessity of multimaterial analysis in certain situations, e.g., the air/product gas interface for a chemical explosive or problems involving water.

This report is meant to summarize the progress made during the period of (approximately) 1987–1990 in developing a particular CFD technology based on a second order adaptation of the ideas of Godunov [33], [34]; also, we discuss the many applications that have been studied using these new methods during this period. The current state-of-the-art is assessed as well.

In order to set the stage for such a discussion, we first summarize the state of affairs in the relevant CFD community at around 1978 when I and others involved in the work here began to look at a certain set of experimental data which did not seem amenable to CFD analysis. At that time, all of the heavily used CFD codes were based on the ideas of the Lax–Wendroff scheme. The aerodynamic community used a relatively clean version – MacCormack's scheme – and were mainly interested in developing, e.g., implicit versions to quickly attain steady state flows. The Defense Nuclear Agency (DNA) community, on the other hand, used codes such as the HULL code which contained a substantially enhanced set of capabilities to enable it to handle the range of phenomonology discussed above; of course, steady state convergence was not an issue. Additionally, many other codes developed at the weapons labs (Los Alamos National Laboratory (LANL) and Lawrence Livermore National Laboratory (LLNL), today) were also used. For example, nuclear weapon design obviously requires multimaterial capability, and this was available since at least the early 1960's. During this period, the first really new method – the Flux Corrected Transport (FCT) scheme developed at Naval Research Laboratory (NRL) – was also being used for unsteady work. A very important observation is that the speed and memory of the pre-CRAY machines were a tiny fraction of the capabilities that we take for granted today; the same can be said for ease of use, post-processing, etc. As a result, it was not possible to make truly high resolution (i.e., in some sense, converged) calculations for difficult problems; hence, it really was not known whether or not the information obtained

from them was reliable. So, just as the aerodynamic community relied mainly on wind tunnels, the DNA community used field tests.

At this time, a new problem arose in the field of high overpressure shock and blast waves. To be precise, experimentalists in both the laboratory and the field were observing, for certain cases, multiple pressure peaks behind the incident wave; the CFD codes were unable to predict the phenomenon and there did not seem to be a viable analytical theory to explain the extra peaks. Simultaneously, three events took place which were to resolve the problem about three years later: (1) the CRAY 1 computer became available, (2) Prof. I. I. Glass at University of Toronto Institute of Aerospace Studies (UTIAS) began using infinite-fringe interferometry in analyzing self-similar laboratory scale shock wave interactions and (3) the second order Godunov scheme was invented by van Leer [64] (and the FCT group was also making rapid progress with related ideas). By 1982, it was completely clear that, at least for the laboratory scale experiments, the extra peak(s) were real and were due to the complexities of double Mach stems. This was independently discovered by the UTIAS interferograms, the FCT calculations and the second order Godunov calculations. At this time, the UTIAS group began a lengthy collaboration with the Naval Surface Warfare Center (NSWC) / Lawrence Berkeley Laboratory (LBL) group which culminated in a direct comparison study (laboratory experiments and calculations) using real (this is obvious for the experiments but difficult for computations because nontrivial equation-of-state (EOS) software must be used) air; the extensive agreement between the two sets of results served to confirm both groups' methods. The computations were performed with a variant of van Leer's MUSCL scheme due to Colella and Woodward [16], [69] as further modified by Colella and Glaz [13]; the latter code was the first with general (convex only, however) EOS capability. The results were published a few years later, see [28], [29]. At this point, the FCT (and even the HULL) results were also confirming the basic ideas. A bit later, another comparison study was undertaken using SF_6 as the test gas, see [30]. Since the assumption of equilibrium is much closer to being correct for SF_6 than for low density air, these comparisons were even better; indeed, they essentially match exactly. In Section 1 below, some further details and new work are briefly discussed for the self-similar case.

Simultaneously with this work aimed at the self-similar case, many groups were now going after high resolution results for height-of-burst studies which are truly unsteady and considerably more computationally expensive. The NSWC/LBL group chose a set of experiments which were carefully analyzed by J. Carpenter. The calculations, which are started by fully burning the appropriate high explosive in an axisymmetric geometry, were performed and analyzed by Colella, et al. [12]. The results matched extremely well with the available data and, more importantly, verified the multiple peak phenomenon; in fact, three distinct peaks at close-in stations were observed in the most highly resolved computation. This, and later CFD work by various groups finally settled the original problem.

At this point, a new set of problems became of interest. An intriguing set of photographs from early nuclear events showed a clear precursor wave moving well out in front of the incident blast wave. Here, an analytic hypothesis could and was formed to explain the phenomenon: radiation heating of the ground and nearby boundary layer air would increase the shock speed near the ground but not too far above it. Also, applications were leading the CFD groups into the study of blast wave phenomena with nonideal boundary conditions and various modeling hypotheses were being tested both experimentally and by calculation. Using the second order Godunov scheme, an idealized setup involving various thermal layers had already been studied by Glowacki, et al. [32] These studies clearly indicated the possibility of thermally induced precursor effects; additionally, the calculations demonstrated the high resolution and accurate computation of multiple vortex rollups and interactions in the very subsonic region well behind the incident shock. This work was to inspire a substantial effort in the study of shear layers during the contract period covered by this report and will be discussed below. In any event, the code was used to simulate nuclear blast events via very long CRAY runs. Some of this work is mentioned in [25] and references therein and it formed the basis for a wide variety of computational simulations which will be one of the subjects of Section 5 below.

Alongside all of these large-scale computations, a revolution was occurring in the CFD community as well as the more theoretically oriented group involved in studying schemes and algorithms. This was largely driven by the exponentially increasing power of the supercomputers, but the influence of the mathematical theory of conservation laws developed by Lax, Glimm, Liu, DiPerna, etc. was also extremely important. Some typical examples of applying these ideas to develop schemes may be found in the references [21], [35], [54], [57], [65]; a particularly useful reference is the review of Yee [70] which contains about 200 references therein. Of course, the high-order, Godunov schemes are the prototypical example of borrowing from the theory of hyperbolic conservation laws. In any event, it is now the case that 1-D gas dynamics problems can be considered solved by at least 20 different variants of the idea of second- or higher-order upwinding.

Additionally, the second-order Godunov technology has been extended in many useful ways since 1985. Examples are the mesh refinement strategy of Berger and Colella [4], the unsplit algorithm of Colella [10] for multidimensional problems and the front tracking method of Chern and Colella [6]. Other examples involving myself are discussed below. At the present time, these efforts are concentrated at LLNL and are being organized by P. Colella and J. Bell.

After a review and update on self-similar oblique shock wave reflection in Section 1, the next three sections discuss progress in various code development projects that I am involved with under this contract. Section 5 lists the many applications that I have been working on with varying degrees of effort during the last three years; since all of this work has been published either in the open literature or as technical reports, it would serve no purpose to discuss the results and so this section is brief. Finally, along with J. P. Collins,

J. Krispin and others, I have involved myself with various aspects of isentropic gas dynamics and testing different algorithms in 2-D settings for these equations; this is the subject of Section 6 which will also be brief since the results will soon be available in preprint form. Related to the work of Section 6, Krispin and myself have undertaken an analogous study of various versions of the second order Godunov scheme as applied to 3-D supersonic steady gas dynamics [40]; 3-D calculations were achieved by operator splitting using the algorithm of Glaz and Wardlaw [31]. Although this work was not funded by DNA, it may still be of interest to some readers.

1.1 SELF–SIMILAR SHOCK WAVE REFLECTION.

Self-similar oblique shock wave reflection for the equations of unsteady inviscid gas dynamics is among the outstanding unsolved problems in nonlinear partial differential equations (PDE). This is so due not only to its standing as the simplest possible nontrivial shock wave interaction problem for these equations and the importance of the problem in engineering applications, but to the tantalizingly large amount of experimental and computational data which is available after half a century of intensive research since WW II.

The equations of unsteady, inviscid gasdynamics in Cartesian coordinates are

$$\rho_t + (\rho u)_x + (\rho v)_y = 0 \tag{1a}$$

$$(\rho u)_t + (\rho u^2 + p)_x + (\rho uv)_y = 0 \tag{1b}$$

$$(\rho v)_t + (\rho uv)_x + (\rho v^2 + p)_y = 0 \tag{1c}$$

$$(\rho E)_t + (\rho uE + up)_x + (\rho vE + vp)_y = 0 \tag{1d}$$

where ρ is the density, $\mathbf{u}$ = (u,v) is the velocity field, E = $\frac{1}{2}(u^2+v^2)+e$ is the total specific energy, e is the specific internal energy, and p is the pressure. The system is closed by specifying an equation-of-state (EOS), p = p(ρ,e); an important example is the polytropic EOS, p = $(\gamma - 1)\rho e$, where $\gamma > 1$ is constant. Equations (1) are a system of conservation laws

$$U_t + F(U)_x + G(U)_y = 0$$

where $U = (\rho, \rho u, \rho v, \rho E)^t$, etc. The initial conditions for oblique shock wave reflection are set up as follows: an incident shock wave, I, of shock wave Mach number M_s traverses an ambient (i.e., $\mathbf{u}_0 = (0,0)$) medium and approaches a wedge surface inclined at θ_w degrees; since the upstream flow is ambient, $M_s = \sigma/c_0$ where σ = shock speed and c_0 is the upstream sound speed. The coordinate system is set by taking the corner at $(x,y) = (0,0)$ and the time $t = 0$ at the instant the shock reaches the corner. There are no length scales in the initial data, the equations (1), or the EOS, so it is reasonable to look for self-similar or pseudosteady solutions for $t > 0$ in the similarity variables

$$(\xi, \eta) = (x/t, y/t). \tag{2}$$

In conservation form, the transformed equations are

$$(\rho\tilde{u})_\xi + (\rho\tilde{v})_\eta = -2\rho \tag{3a}$$

$$(\rho\tilde{u}^2 + p)_\xi + (\rho\tilde{u}\tilde{v})_\eta = -3\rho\tilde{u} \tag{3b}$$

$$(\rho\tilde{u}\tilde{v})_\xi + (\rho\tilde{v}^2 + p)_\eta = -3\rho\tilde{v} \tag{3c}$$

$$(\rho\tilde{u}\tilde{H})_\xi + (\rho\tilde{v}\tilde{H})_\eta = -\rho(\tilde{u}^2 + \tilde{v}^2) - 2\rho\tilde{H} \tag{3d}$$

where $\tilde{\mathbf{u}} = (\tilde{u}, \tilde{v})$ is the self-similar velocity field, $\tilde{u} = u - \xi$, $\tilde{v} = v - \eta$, $\tilde{H} = \frac{1}{2}(\tilde{u}^2 + \tilde{v}^2) + h$ is the self-similar total enthalpy, and $h = e + p/\rho$ is the specific enthalpy. Additionally,

$$\tilde{M}^2 = (\tilde{u}^2 + \tilde{v}^2)/c^2 \tag{4}$$

defines the self-similar Mach number $\tilde{M}$, where c = sound speed. In vector form, the equations (3) are written

$$\tilde{F}_\xi + \tilde{G}_\eta = \tilde{S}$$

where $\tilde{F} = (\rho\tilde{u}, \rho\tilde{u}^2 + p, \rho\tilde{u}\tilde{v}, \rho\tilde{u}\tilde{H})^t$, etc. One notes that the first-order part of this system, $\tilde{F}_\xi + \tilde{G}_\eta = 0$, are exactly the equations of steady gas dynamics in the (ξ, η) coordinates.

The wall boundary condition for equations (1) is perfect reflection, i.e., flow is parallel to the wall. It is easily seen that this condition transforms analogously for equations (3). The boundary condition at infinity for equations (1) is the time-dependent Dirichlet condition provided by the Rankine-Hugoniot conditions connecting states U_0 and U_1. Since no disturbance can reach infinity in finite time, this boundary condition can also be easily transformed. Further, the boundary may be moved to a finite distance from the origin so long as it is outside the region of disturbed flow; the intersection of the incident shock with such a boundary is easily calculated in the (ξ, η)-frame for $t > 0$ by using the known shock speed, σ.

Unlike equations (1), which are always hyperbolic under very general conditions on the EOS, the equations (3) of steady gas dynamics with source terms are hyperbolic only when the flow is supersonic in the (ξ, η)-frame. For subsonic flow, the streamline characteristic remains real but the sound wave characteristics become complex. Thus, equations (3) are of mixed type. Note, however, that for the boundary conditions under consideration here, the flowfield becomes supersonic as $(\xi, \eta) \to \infty$ for any initial data; in particular, any finite farfield boundary chosen as above should satisfy the condition that the flow is supersonic nearby.

Summarizing, we are interested in solving the boundary value problem given by equations (3) subject to the given boundary conditions. Evidently, the solution depends parametrically on M_s, θ_w, the EOS and the ambient data (ρ_0, e_0). For the important case of a polytropic gas, the parameters are M_s, θ_w and γ; the ambient state is no longer an independent parameter. To the best knowledge of the author, there do not exist any mathematical results pertaining to the question of global solutions for this problem; the issues of existence, uniqueness, and continuous dependence on the parameters remain open for all parameter ranges.

Any conjectures that we have concerning these questions must be inferred from shock tube experiments and CFD simulations. Additionally, mathematical analysis is often applied to infinitesimal or local flowfield regions, especially shock wave interactions, once such regions are apparent from experiments or calculations. Of course, such experiments and calculations are subject to experimental error (e.g., the incident shock has a finite

thickness and may not move at precisely constant speed, the wall will not be perfectly smooth, data analysis errors, etc.) and numerical error. Also, any experimental result will represent a solution, not of equations (1), but of an augmented version of equations (1) which takes into account real gas effects such as vibrational relaxation, dissociation-recombination chemistry, and viscosity. In some examples (especially at high M_s), these effects are significant; in all cases, it is necessary to carefully analyze them. Numerical simulations may not be fully resolved, may introduce 'artificial' viscosity, and may contain other systematic errors; furthermore, it is not possible to prove convergence or obtain useful error estimates at the present time. Despite all of these caveats, most workers in the field would at least maintain that the data is very useful in deducing properties of solutions of equations (3). Still, it must be emphasized that the answers to these questions are not at all obvious.

For further analytical/mathematical analysis of self-similar oblique shock wave reflection, the reader may find [26] useful. Recently, several review articles on this subject have appeared; we mention those by G. Ben-Dor [3], I. I. Glass [23] and H. Hornung [39]. These references also lead to many hundreds of papers in the field. We single out the very important work of L. F. Henderson, et al. [36], [37], [38] on the subject of transition between regular and Mach reflection which is the outstanding open question.

As noted in the Introduction, this problem has been the subject of many numerical studies. This is due not only to it's inherent interest, but also to it's suitability as a difficult test problem for numerical methods. The earliest work of this type dates back to the mid-1970's and was done in the aerospace CFD community; see [51], [58] and [59].

An extension of the basic second order Godunov technology was developed for the high M_s cases where real gas effects in low density air lead one to suspect that the flowfield is not in equilibrium (and, therefore, is not self-similar since the relaxation times introduce new scales into the equations). The results were finalized and appeared in the open literature during the contract period, see Glaz, et al. [27]. These new calculations were all that we could have hoped for since they explained away all of the quantitative disagreements discussed in the precedent work [28], [29] where nonequilibrium effects were conjectured to be decisive. It may also be mentioned that a code of this type, adapted for general geometries, would be quite useful in high altitude aerospace studies.

Finally, a very nice numerical study of the weak limit case has been undertaken by Colella and Henderson [14]. The numerical results therein seem to have resolved some of the open questions among the large subcommunity interested in this problem.

1.2 A NEW PROJECTION METHOD FOR INCOMPRESSIBLE FLOW.

Around 1968, A. J. Chorin and R. Temam developed projection methods for the incompressible Euler and Navier–Stokes equations. This is an inherently split method in which the advection or advection–diffusion step takes the velocity field out of the space of divergence–free vector fields (this may be thought of either at the PDE level or at the discrete level with suitable discrete divergence and gradient operators) and the projection step calculates the divergence–free part of this field. Of course, this is a linear algebra problem. Bell, et al. [1] have updated this algorithm in three ways: (1) the linear algebra has been significantly modernized, (2) the coupling between the two split steps is stronger and (3) the advection algorithm has been radically altered from a standard finite difference to a version of the unsplit second order Godunov scheme. The latter step has led to spectacular improvements in the resolution capabilities of the method.

Further work in extending the algorithm for the Boussinesq approximation, fully variable density flow and 3-D versions is continuing at LLNL by J. Bell and colleagues. Ultimately, the method may be able to handle the low–speed part of fireball calculations and couple with a compressible algorithm at some point for the late stages. In this sense, it is a competitor for the implicit–explicit technology discussed in Section 3. Also, it has occurred to many of us that the zero Mach number limit of the latter algorithm may well be a version of the new projection algorithm and that understanding this limit may be the key to obtaining sharp estimates on the performance of both scheme classes.

1.3 IMPLICIT–EXPLICIT SCHEMES.

A hybrid implicit-explicit scheme of a type first discussed in [22] for the case of Lagrangian hydrodynamics has been developed for the equations of Eulerian hydrodynamics by Collins, et al. [18]. For these schemes, the difference approximation in time is either implicit or explicit, separately for each family of characteristics and for each cell in the finite difference grid, depending on whether the local CFL number for that family is greater than or less than one. In both cases the hybridization is continuous at CFL number equal to one, and the scheme for the explicit modes is a second-order Godunov method of a type discussed in [16], [13].

This implicit–explicit strategy is intended for problems with spatially and/or temporally localized stiffness in wave speeds. By stiffness, we mean that the high speed modes contain very little energy, yet they determine the explicit time step through the CFL condition. For hydrodynamics, the main example is nearly incompressible flow. Here, the sonic waves will be nearly acoustic and largely decoupled from the particle modes. Traditionally, such problems are handled in one of two ways: at the PDE level by solving instead the incompressible limit of the set of governing equations, or numerically by artificially increasing the temperature of the gas in such a way that the Mach number becomes significant but still low enough that compressibility effects are negligible.

Another example is provided by magnetohydrodynamic calculations in certain configurations [5], [56]. Here, if the problem leads to spatially localized regions where a low density plasma is immersed in a strong magnetic field then the Alfvèn wave speed can become very large. Our approach can potentially deal with this problem in a straightforward manner and avoid ad hoc solutions, e.g., modifying the calculation of the electric field at low densities.

A related example is the problem of shock wave – boundary layer interaction. It is often important to simultaneously perform a high resolution calculation of the strong wave interactions in the free stream while also resolving enough of the detail in the boundary layer to accurately model the effect of the no–slip boundary condition on the free stream as well as handling any transport effects between the boundary and the inviscid flow region (which might include particle and temperature transport from the boundary condition). The boundary layer length scale is usually several orders of magnitude smaller than even a single computational zone width, while the particle speed is approaching zero along with the strengths of the sonic waves as the boundary is approached. These difficulties can be partially ameliorated by constructing appropriate adaptive meshes, but this is not usually sufficient. A common approach, especially in engineering calculations where efficiency is important, is not to use boundary layer zoning at all but to explicitly difference some approximation to the Navier–Stokes equations in the first several zones near the boundary, thereby satisfying the correct boundary condition. Of course, accuracy can be a problem in such calculations. Alternatively, one can use boundary layer zoning at the expense of also differencing the entire set of equations implicitly, at least in a locally refined region,

in order to avoid stability problems; a discussion of such methods for upwind schemes may be found in [70]. Potentially, the latter approach is viable, but the interface between the boundary layer and inviscid regions can be a difficult numerical problem. The extension of our approach to the Navier–Stokes equations, also developed in [18], allows for the smooth transition between a high resolution explicit scheme in the exterior flowfield and a stable method in the boundary layer.

The development of our implicit–explicit scheme has followed the following design principles:

(1) The scheme is in conservation form, both for conservation laws and for their viscous extensions.

(2) The implicit–explicit hybridization is a continuous switch and operates on each characteristic field separately; the method is entirely local in both time and space, depending only on the data in each computational zone.

(3) In the event that all characteristic modes are explicit, the scheme reduces to a version of the second order Godunov scheme [16], [13].

(4) The implicit advection scheme, which is only first order accurate in time, satisfies a maximum principle and is unconditionally stable.

(5) In the limit of steady state, the scheme is second order accurate in space.

The first three of these properties are satisfied by the scheme of Fryxell, et al. [22]. Their implicit scheme is also second order accurate in time, but does not satisfy a maximum principle (and, therefore, is not monotone). Additionally, for a system of n equations, their method requires the inversion of a block $2n \times 2n$ tridiagonal system whereas the current method requires only a block $n \times n$ tridiagonal system. For our intended applications, we do not regard the lack of second order temporal accuracy to be a serious problem. Waves that we wish to resolve in a flowfield will be treated using the second order accurate explicit scheme; the others will be rapidly relaxed to equilibrium.

A key component of the work described in [18] is the introduction of an appropriately smooth numerical flux function for the hyperbolic equations. We use a suitable version of the Engquist–Osher flux [21] as modified for systems by Bell, et al. [2]. The version used is sufficiently smooth so that the Newton's method linearization is well-behaved; in particular, it converges to steady states even in the presence of strong shocks.

The special case of one-dimensional inviscid and viscous compressible flow is treated in [18] and a polytropic equation-of-state is assumed for convenience. However, the ideas and implementation methodology are easily extended to more general systems in one space dimension. In particular, it is expected that our results can be extended to gas dynamics with a general equation-of-state using the ideas in [13]. A more difficult question is the extension of these ideas to two or three space dimensions. A few operator split 2D boundary layer calculations have already been successfully completed by Collins [17].

At the present time, Collins is attempting to develop an unsplit version of the method-

ology using the explicit unsplit, second-order Godunov scheme introduced by Colella [10] as a starting point; this work, if successful, will lead to his Ph. D. degree in Applied Mathematics at the University of Maryland, College Park (I am his thesis advisor). Our strategy is to concentrate first on the zero Mach number limit for gas dynamics with periodic boundary conditions; as noted in Section 2, this approach may well lead to significant new ideas in several directions. In addition, we are experimenting with alternatives to Newton linearization such as multigrid acceleration and preconditioned conjugate gradients applied to the discrete nonlinear problem for the implicit modes. Later, nontrivial boundary conditions will be introduced along with various approximations of the viscous terms in the Navier–Stokes equations so that boundary layer transport can be calculated. Ultimately, some version of mesh refinement will be required so that the full Navier–Stokes equations can be solved in critical regions, e.g., the reflection point in studies of transition between regular and Mach reflection. When this point is reached, it is fortunate that experimental work from UTIAS will be available which may well be useful in validating and/or improving the algorithm; we refer to the papers [61], [62], [66] in which transition was studied as a function of Reynolds number.

1.4 MULTIMATERIAL ALGORITHMS.

Colella, et al. [11], have developed a volume-of-fluid type method for the numerical calculation of compressible flow problems in which the fluid is made up of a number of thermodynamically distinct materials separated by sharp interfaces. In this approach, a standard finite difference representation of the solution is augmented by cell-centered values for the thermodynamic quantities: ρ^α, e^α, V^α, are the density, internal energy, and fractional volume occupied by the α^{th} fluid in each zone, $\alpha = 1, \dots, n_f$. The evolution of this representation can be thought of as consisting of two parts. One is the effective Lagrangian dynamics—the accelerations, compressions, and work done on the multifluid representation—which is computed under the assumption that the various fluid components are in pressure equilibrium with one another in each cell, and that each cell has a single velocity. From a physical point of view, the assumption of pressure equilibrium is not unreasonable, since the pressure is continuous across a contact discontinuity. The requirement that the cell has a single velocity is not an appropriate one in more than one dimension, since slip can be generated at a fluid interface. Thus, the jump in the thermodynamic variables across the interface is tracked, while the jump in tangential velocity is captured using the underlying conservative finite difference method. The other part of the evolution is the motion of the fluid-interface through the finite difference grid. This is done by reconstructing locally the interface geometry from the fractional volumes, and transplanting material along streamlines defined by the single fluid velocities. Multifluid methods have been in use for some time as noted in the Introduction and have been quite effective in representing complicated multifluid configurations undergoing large distortions.

Two innovations into this class of algorithms are introduced in [11]. The first one concerns the effective Lagrangian dynamics of the multifluid cells. A formulation of this dynamics which is thermodynamically consistent is derived there. If the various fluid components in a cell are in pressure equilibrium, then they remain so to leading order in the truncation error, assuming the the pressure gradients and compressions are finite. Since that assumption will occasionally be violated–for example, when a shock over-takes a material interface–a relaxation scheme to restore pressure equilibrium in multifluid cells is introduced. The second innovation is the coupling of this method to an operator-split, second-order, Eulerian, Godunov method. In previous multifluid algorithms, the conceptual division into two parts was used literally as the basis for the design of the algorithm, with the underlying single-fluid algorithm having to be formulated as a Lagrangian step followed by a remap. In the approach taken in [11], the underlying difference algorithm is a conservative predictor-corrector method which provides pressures and velocities at the cell edges as part of the flux calculation.

Both 1-D and 2-D calculations are presented in [11]. In fact, 2-D supersonic jets have been very successfully calculated with previous versions of the algorithm (in a few cases, the results indicated new physics not previously calculated by others working the same problem – a set of models based on astrophysical jets). A key change in the new version is

a slight modification in the technique used by the underlying single fluid algorithm in it's handling of general EOS. This change has enabled us to perform HE product gas/water calculations using the Gittings EOS for water. It is hoped that the new scheme will find applications in this environment for the DNA community.

Finally, a very successful study has been undertaken by Colella et al [15] in simulating several cases of shock wave refraction and, in some runs, comparing with experimental work of L. F. Henderson. These calculations were based on a version of the algorithm presented in [11].

1.5 APPLICATIONS.

A major effort has been undertaken over the past five years in studying free shear layers in an attempt to prove that instability and rollup is a purely inviscid dynamic phenomenon and is independent of the Reynolds number, see [7–9] and, especially, [43]. I believe that our simulation of the famous Brown–Roshko experiment of 1974 which is reported in great detail in [43] is the best calculation ever made using the old split version of the second order Godunov scheme. It is clear that major contributions have been made to this area of fluid mechanics.

The reports [42], [44–50] detail the many calculations performed from NSWC over the past few years in studying wall bounded shear layers and jets, precursors and decursors for both simulations and airblast modeling and gas–particle 2–phase boundary layer modeling under the restraints involved in using an inviscid code. Dense gas models were used as well as the dusty gas limit model, see [53]. Many of these calculations were very large–scale, involving massive data sets and complex postprocessing and analysis.

Finally, I was involved in a demonstration study using the new quadrilateral unsplit code developed at LLNL; we set up various loading configurations already studied experimentally at UTIAS and made several very successful comparison calculations [24]. Currently, we are now redoing these runs using the even newer quadrilateral AMR code; the preliminary results are quite spectacular and we would like to finish this study soon. The reader may be interested in earlier loading calculations using the operator split version of the code; see [25] and references therein.

1.6 ISENTROPIC GAS DYNAMICS.

The equations of 2D unsteady isentropic gas dynamics are given by equations (1a), (1b), and (1c) of Section 1 with the EOS given by the relation $p = p(\rho)$. Just as for gas dynamics, this set of equations forms a system of hyperbolic conservation laws

$$U_t + F(U)_x + G(U)_y = 0$$

where $U = (\rho, \rho u, \rho v)^t$, etc. This effectively replaces the energy equation by the constraint that the entropy be conserved along streamlines; in practice, we have assumed that the entropy is everywhere a constant. These equations are valid in two limiting situations. First, since the jump in entropy across a discontinuity is of third order in the shock strength and entropy is conserved in smooth flow, this set is an excellent approximation if all shocks may be assumed to be weak a priori. Also, the system is equivalent to a version of nonlinear acoustics if the variables are reinterpreted appropriately. The same is true for the shallow water equations. Second, the entropy jump is small, even for very strong waves, if the material density is large and the EOS is stiff; the example of interest here is shock loading of metals although some of the ideas may also be useful for water.

In one space dimension the fluid dynamic equations are equivalent to the equations of solid mechanics in their simplest formulation with the exception that the pressure is viewed as the stress but of opposite sign; of course, the constitutive modeling (i.e., the EOS here) may be more difficult. Some materials, such as iron and Plexiglas, undergo a phase change when shocked to a sufficiently high pressure. To model this phenomenon, it is necessary to allow the EOS to be non-convex in the appropriate pressure ranges; the theory of hyperbolic conservation laws predicts more complicated wave structures in this case. This theory, in particular as it applies to the Riemann problem, is well understood and agrees with results from experiment for those few situations where such experiments are possible. A major objective of our work was to simulate the $\alpha - \epsilon$ phase transition in Iron which occurs at about 137 kilobars and has been extensively studied. Our model is too simple to allow for the weak elastic precursor wave which is observed in some experiments but this has not been a major factor; an interesting point is that this precursor wave is much faster than the following main wave pattern and, if we had included it in our model, the implicit–explicit ideas of Section 3 would be useful.

Another objective of this work was to test several variants of the second-order Godunov scheme in the relatively simple setting of isentropic gas dynamics, but for materials where the solution to Riemann problems would be complex and very expensive to compute exactly. This comparison study was based on three approaches: the original algorithm of Colella and Glaz [13] suitably adapted for the EOS, the very general methodology of Bell, et al. [2] (which is referred to below as the BCT method) and an extremely simple version due to Davis [20]. We worked with a model EOS as well as the iron EOS from the literature and 1D and 2D problems were studied. The 2D calculations were the analogue of the oblique self-similar shock wave reflections discussed in Section 1 for the equations

of isentropic gas dynamics, although here we have no experimental data against which to compare.

The results of this work are detailed in the paper of Krispin, et al. [41]. A very brief summary follows. First, the new phenomenology resulting from the nonconvexity is quite exciting and it would be of interest to see if similar results are in the experimental literature. From the numerical point of view, the original algorithm worked quite well and was very expensive, as expected. The Davis approach is reasonable for simple solutions such as regular reflection but appears to break down when there are strong 2-D wave interactions, e.g., double Mach reflection; on the other hand, it is a very efficient method. The main conclusion was that several variants of the BCT method yielded excellent quality results at an intermediate, but acceptable, expense. We believe that this type of study will become more common in the field as shock waves in exotic materials and more complicated systems of conservation laws are modeled numerically.

Another study has also been carried out with the same code for the simpler case of a convex EOS. Here, we were working from a set of conjectures concerning possible solutions of the two-dimensional Riemann problem for isentropic gas dynamics. The initial data was chosen from the special cases in which each of the four one-dimensional Riemann problems has a solution consisting of one wave only; still, the analytic problem is quite formidable. The general case is surely impossible to solve other than by numerical means so our efforts here are partially a validation study for a future attack on the general case. The results have been collated and analyzed with respect to the a priori conjectures, see Collins, et al. [19]. They may be stated quite simply: (1) some of the conjectures are true and others are false and (2) many of the wave interaction patterns are quite striking. Indeed, it is possible to recover all of the self-similar wave patterns familiar from the studies mentioned in Section 1 through judicious choice of initial data.

SECTION 2
CONCLUSIONS

I believe that the following conclusions are quite clear:

(1) The older operator split code for gas dynamics with a general convex equation of state along with the many driver programs written to use it (e.g., blast wave, wedge, simulator, shear layer, etc. drivers) is extremely robust and, if not pushed too far, reliable. The results obtained, both for theoretical physics studies as well as for engineering applications, are clearly the equal or better than those obtained with competing CFD technologies.

(2) The more recently developed versions which include mesh refinement capability, general quadrilateral meshes, etc. have extended the range of problems which we can study as well as improve our studies for problems for which both the older and newer methods are applicable in the sense that higher resolution can be obtained more efficiently (however, this is not always the case).

(3) The implicit–explicit methodology has passed it's initial testing and it seems likely that a general capability will be available in a few years for several types of problems of great interest to the DNA community. The relationship between this idea and the new version of the projection code for incompressible flow may prove to be the theoretical key in making fast progress.

(4) The multimaterial extension of the second order Godunov scheme is now available for 2-D problems, at least for gases where it has been validated against experimental data and, in a different set of computations, has compared favorably with other numerical studies. The more difficult case of gas–water interfaces is decidedly more promising than even a year ago and it appears that 2-D applications will be feasible with a little additional work.

(5) Our studies on isentropic gas dynamics have indicated that a great deal of fundamental work remains to be done in the area of numerical schemes for situations involving unusual wave pattern phenomenology. These problems – e.g., solid mechanics, multiphase flow, MHD, etc. – are coming under increasing scrutiny in the mathematical community and it seems that the DNA community has substantial applications in these fields. It should also be emphasized that the phenomenology is of interest in its own right.

SECTION 3
RECOMMENDATIONS

(1) A greater effort should be made to make proven codes such as the original operator split, second-order Godunov code for general convex EOS available to the community at large. I do not recommend making drivers freely available except on a case-by-case basis. The same goes for new ard/or experimental codes.

(2) I strongly support DNA's efforts at the central site in the area of graphics support.

(3) It seems that personal workstations are becoming more powerful at an accelerating rate; DNA applications may soon be possible on such equipment. On the other hand, it may become increasingly possible to perform 3-D computations on massively parallel machines (although I believe that this possibility is being overrated in the near term, at least in terms of solving significant problems such as transition and secondary transition to 3-D turbulence followed by highly resolved simulations of the resulting fully turbulent flowfield). Thus, it is at least possible that CRAY equipment may be squeezed from both ends. This should be studied in about two years and resolved soon thereafter from the point of view of DNA interests.

(4) The very substantial code development efforts, centered at LLNL, have paid off in many important ways and should be continued. I believe that the further study of the implicit-explicit idea is highly warranted in view of the large payoff if it works out.

(5) Somebody should find out whether or not second-order Godunov schemes work on triangular meshes (by which I mean general and, preferably, moving meshes, and not simply subdivisions of rectangular meshes for which special treatments are clearly possible).

(6) Shock waves in multiphase flow is a very interesting mathematical problem as evidenced by the work of Wendroff [66–67] and see also [55]. A study should be made to determine whether or not numerical scheme development is warranted in this area relative to DNA interests. On the other hand, it is obvious that codes are required for multiphase boundary layers and I very strongly recommend that our efforts aimed at this goal be continued.

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